

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
 Data File : BF142404.D
 Acq On : 15 May 2025 21:05
 Operator : RC/JU
 Sample : Q2022-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COMP-1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142404.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.110	488	496	508	rBV	181550	264599	9.56%	1.051%
2	5.510	558	564	569	rBV	1606264	2067855	74.72%	8.214%
3	6.516	729	735	740	rBV	1731218	2295365	82.94%	9.118%
4	6.898	795	800	805	rBV	721872	888523	32.10%	3.529%
5	7.457	889	895	900	rBV	1092069	1379583	49.85%	5.480%
6	7.710	934	938	949	rVB	32417	41565	1.50%	0.165%
7	8.181	1013	1018	1032	rBB	927012	1165310	42.10%	4.629%
8	9.257	1195	1201	1206	rBV	2228969	2767633	100.00%	10.994%
9	9.798	1289	1293	1298	rBV	30364	39099	1.41%	0.155%
10	9.934	1311	1316	1322	rBV	1013707	1304178	47.12%	5.181%
11	10.651	1432	1438	1444	rBV	429350	556707	20.11%	2.211%
12	10.722	1445	1450	1461	rBV	1422669	1818742	65.71%	7.225%
13	10.845	1466	1471	1478	rVB2	30185	51263	1.85%	0.204%
14	10.957	1486	1490	1497	rVB2	33713	42014	1.52%	0.167%
15	11.316	1548	1551	1556	rVB2	19203	28680	1.04%	0.114%
16	11.422	1564	1569	1577	rBV2	990231	1392780	50.32%	5.532%
17	11.945	1650	1658	1669	rBV2	237368	461269	16.67%	1.832%
18	12.033	1669	1673	1675	rBV2	53318	70569	2.55%	0.280%
19	12.122	1683	1688	1692	rBV3	23399	38430	1.39%	0.153%
20	12.222	1699	1705	1707	rBV2	29330	49968	1.81%	0.198%
21	12.475	1744	1748	1751	rBV	42102	45341	1.64%	0.180%
22	12.504	1751	1753	1759	rVB2	28835	42454	1.53%	0.169%
23	12.557	1759	1762	1771	rVB4	26834	42560	1.54%	0.169%
24	12.633	1771	1775	1780	rBV	132656	172793	6.24%	0.686%
25	12.727	1788	1791	1795	rBV	36642	48906	1.77%	0.194%
26	12.863	1809	1814	1820	rBV	207410	294273	10.63%	1.169%
27	13.010	1833	1839	1846	rVB	2013388	2569010	92.82%	10.205%
28	13.080	1847	1851	1858	rBV2	38181	73627	2.66%	0.292%
29	13.175	1863	1867	1873	rVV4	38238	81908	2.96%	0.325%
30	13.239	1874	1878	1884	rVV3	22720	41526	1.50%	0.165%
31	13.298	1884	1888	1895	rVB	44423	61126	2.21%	0.243%
32	13.386	1900	1903	1906	rVV	36533	47628	1.72%	0.189%
33	13.416	1906	1908	1912	rVB	29660	35263	1.27%	0.140%
34	13.580	1932	1936	1944	rVB5	20767	48047	1.74%	0.191%
35	13.698	1952	1956	1964	rVB	33684	48682	1.76%	0.193%
36	13.810	1970	1975	1978	rBV3	31824	58873	2.13%	0.234%

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Stop Thrs : 0

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 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	13.910	1987	1992	2002	rVB	138996	231170	8.35%	0.918%
38	14.063	2011	2018	2029	rBV2	794090	1302267	47.05%	5.173%
39	14.222	2039	2045	2053	rVB4	43481	100731	3.64%	0.400%
40	14.451	2075	2084	2086	rBV	46928	93211	3.37%	0.370%
41	14.480	2086	2089	2093	rVB3	31097	32600	1.18%	0.129%
42	14.533	2093	2098	2103	rBV2	200969	371312	13.42%	1.475%
43	14.845	2148	2151	2155	rVB	39389	50232	1.81%	0.200%
44	14.998	2172	2177	2188	rVB4	96392	198675	7.18%	0.789%
45	15.116	2192	2197	2205	rVV2	66694	156606	5.66%	0.622%
46	15.192	2205	2210	2221	rVB	350224	546400	19.74%	2.170%
47	15.421	2245	2249	2254	rVB	51699	72779	2.63%	0.289%
48	15.486	2255	2260	2265	rVV	51468	78983	2.85%	0.314%
49	15.551	2265	2271	2284	rVB	518827	855633	30.92%	3.399%
50	15.792	2307	2312	2323	rVB	88014	151299	5.47%	0.601%
51	16.039	2347	2354	2360	rBV	179043	323989	11.71%	1.287%
52	16.863	2488	2494	2504	rBV4	38952	88041	3.18%	0.350%
53	17.045	2520	2525	2532	rBV2	17387	36524	1.32%	0.145%
54	17.498	2597	2602	2611	rVB	21076	47964	1.73%	0.191%

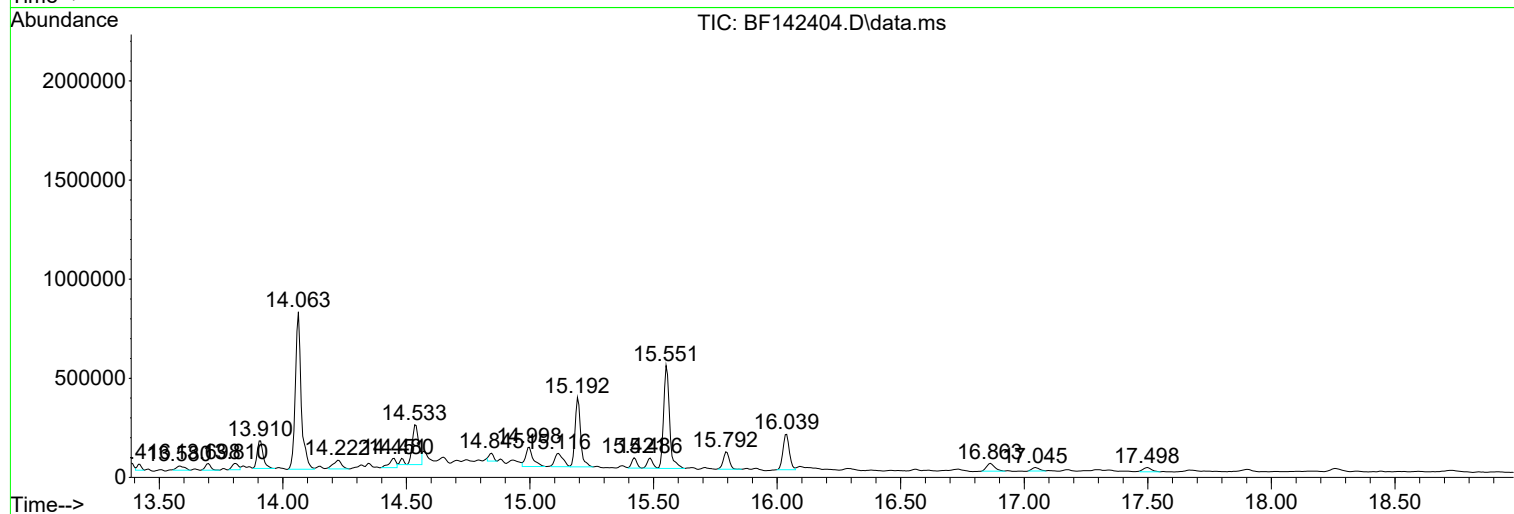
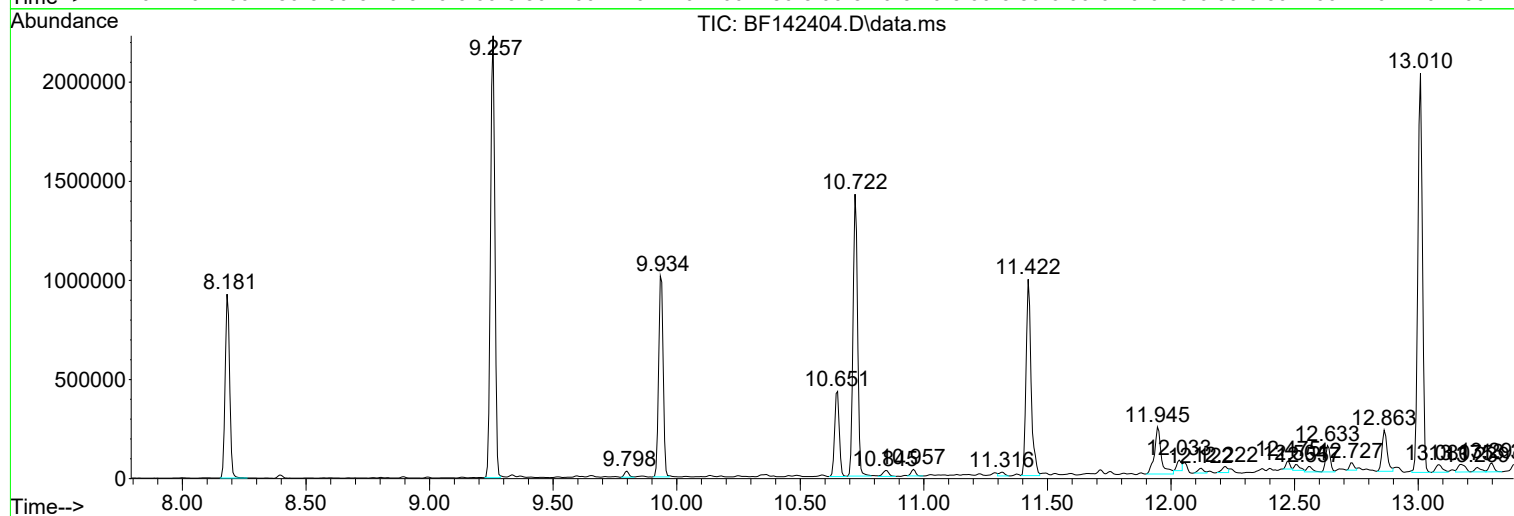
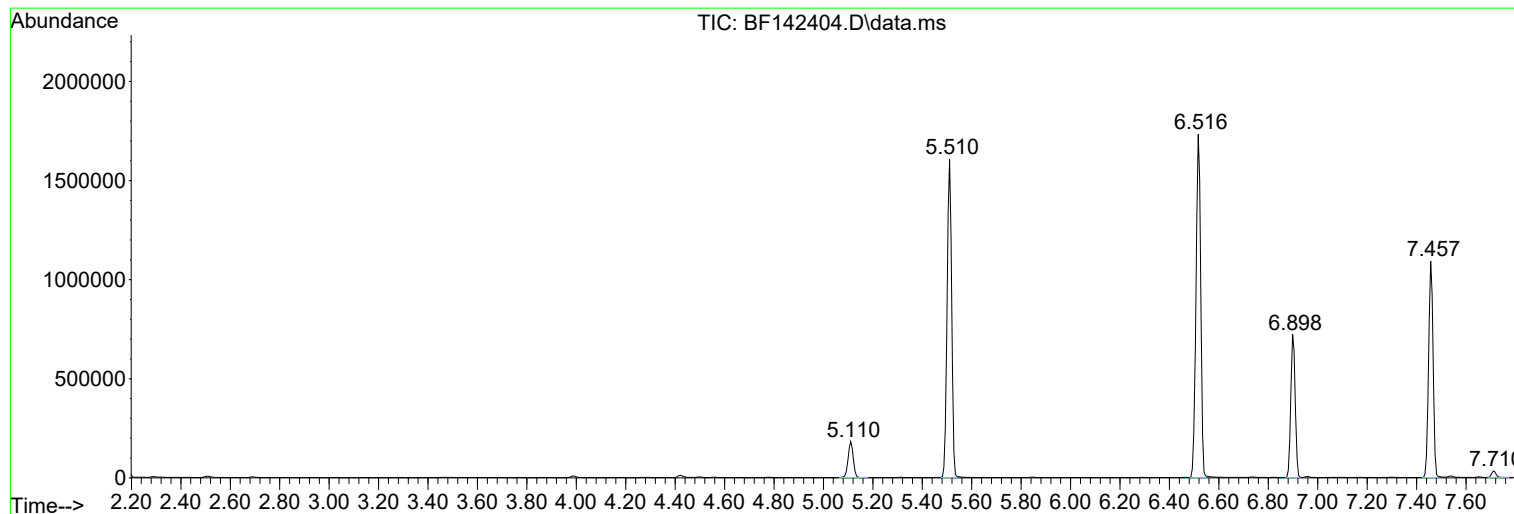
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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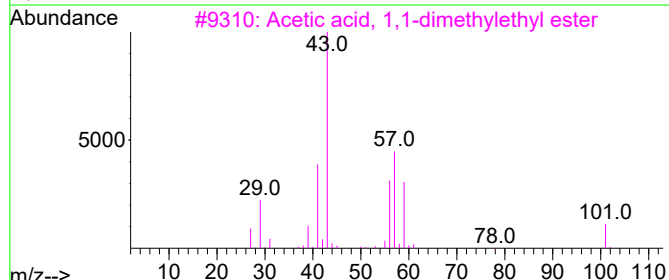
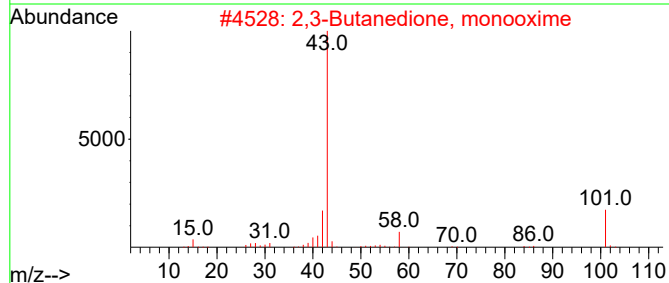
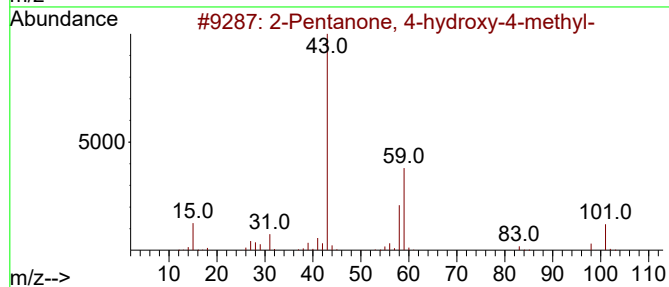
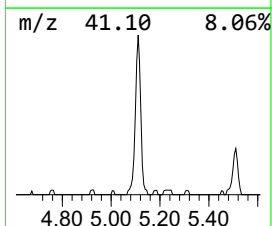
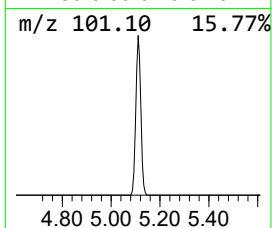
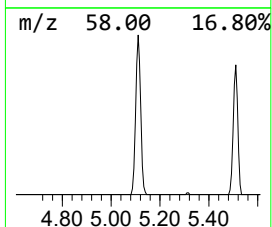
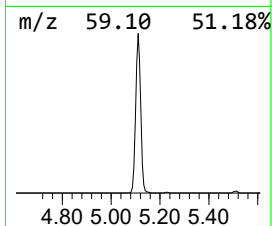
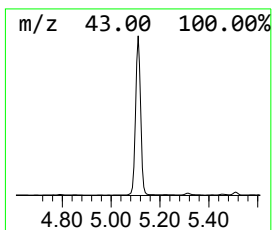
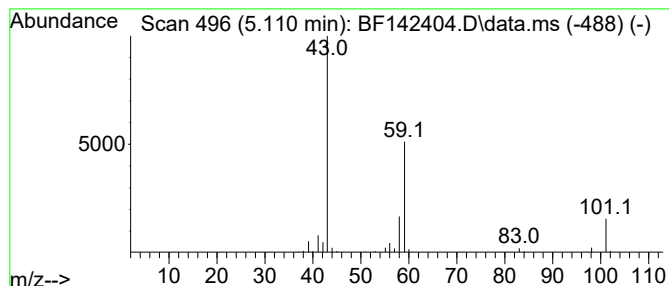
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.96 ng	264599	1,4-Dichlorobenzene-d4	6.898

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	23
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9



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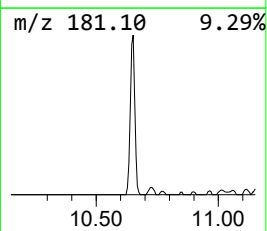
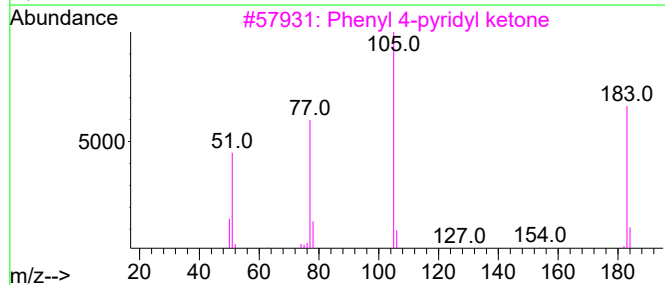
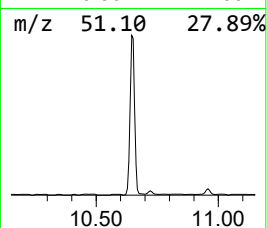
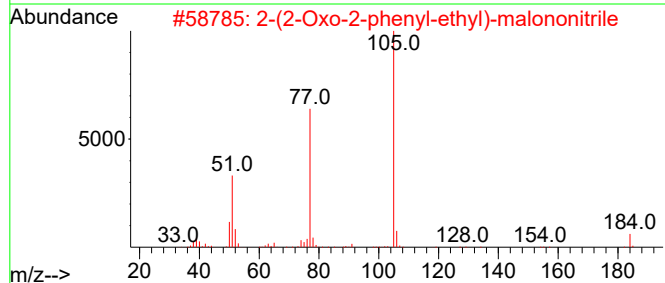
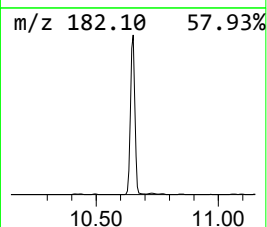
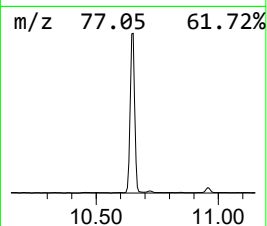
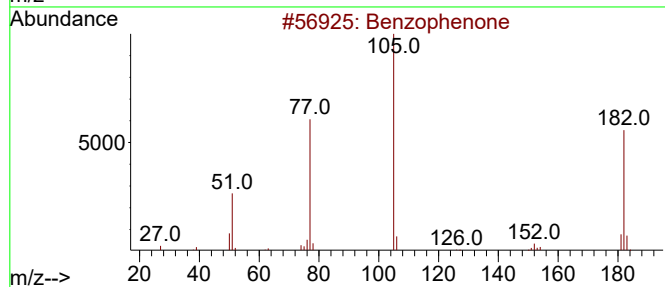
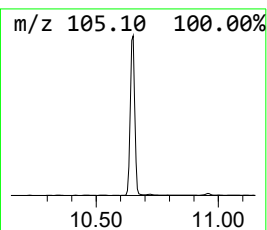
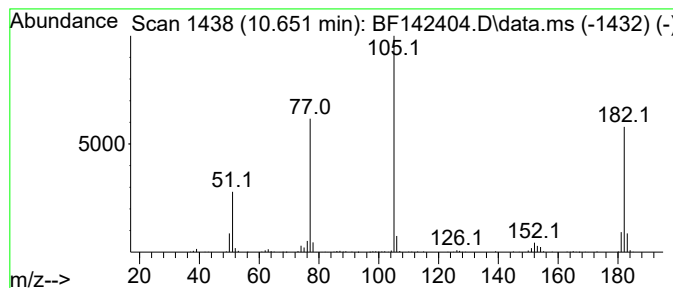
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.651	8.54 ng	556707	Acenaphthene-d10	9.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	53
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	49
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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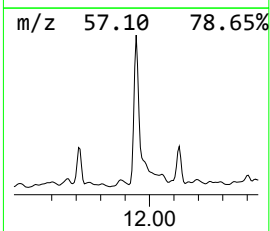
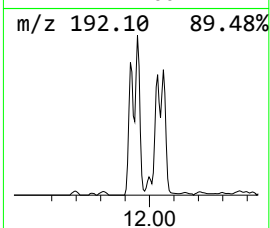
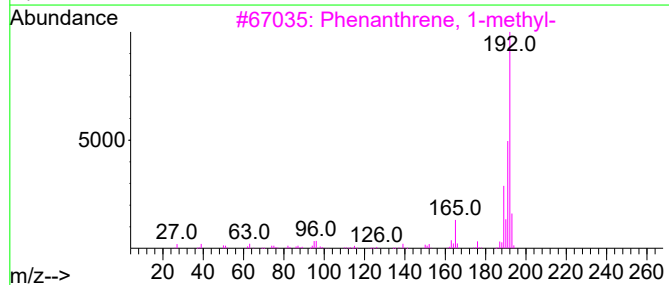
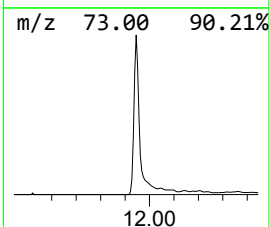
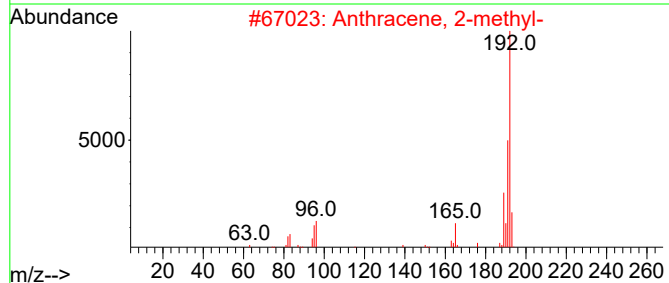
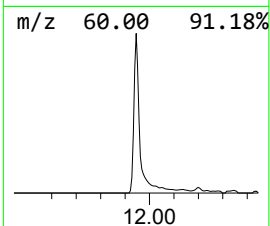
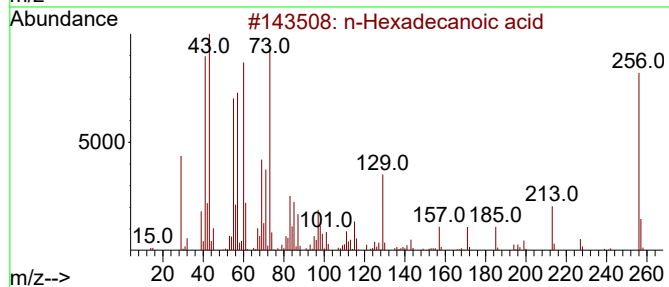
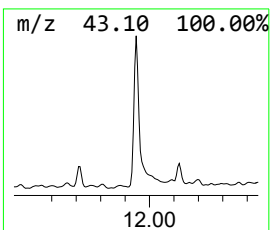
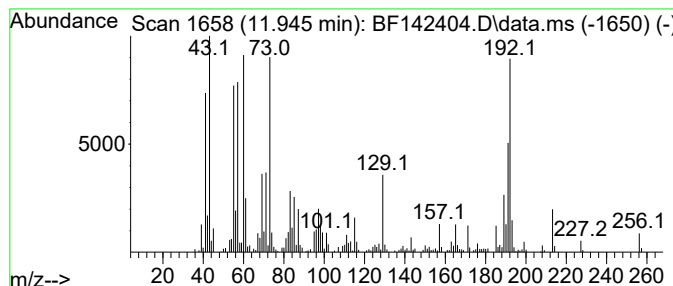
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	6.62 ng	461269	Phenanthrene-d10	11.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Anthracene, 2-methyl-	192	C15H12	000613-12-7	94
3			Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	92
4			Phenanthrene, 2-methyl-	192	C15H12	002531-84-2	92
5			Tridecanoic acid	214	C13H26O2	000638-53-9	89



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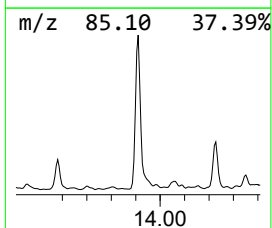
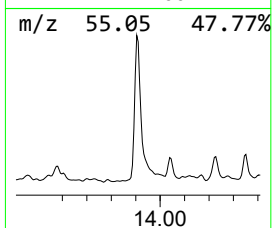
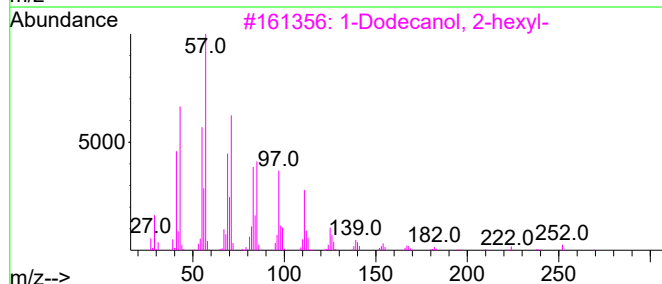
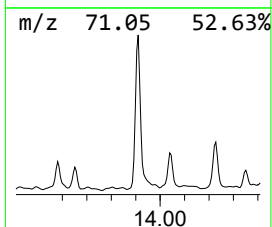
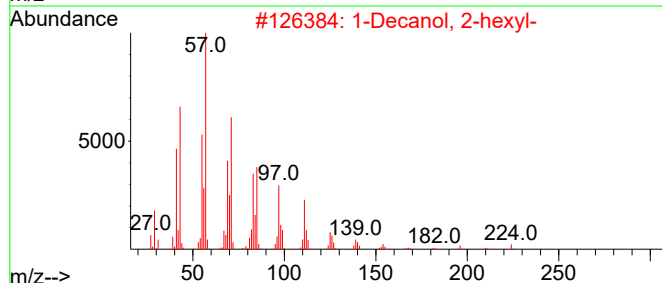
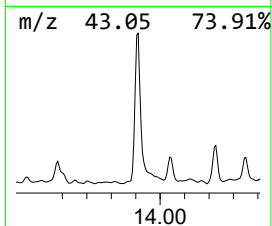
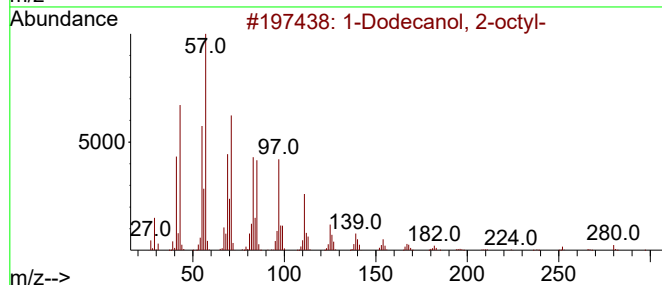
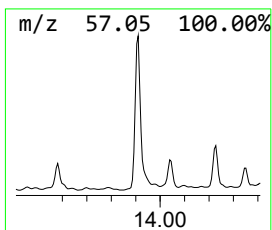
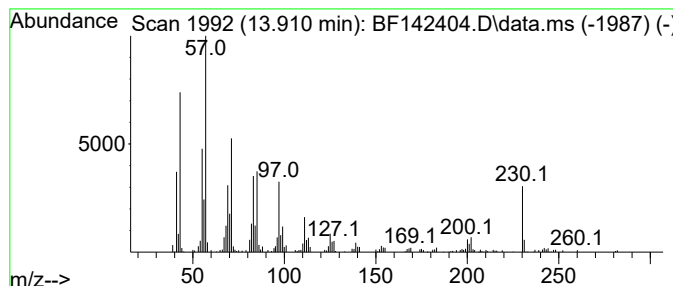
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Dodecanol, 2-octyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	3.55 ng	231170	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	87
2			1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	87
3			1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	87
4			Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	87
5			Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	76



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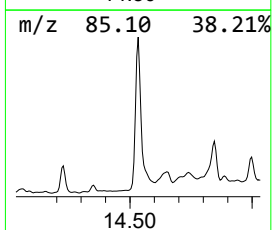
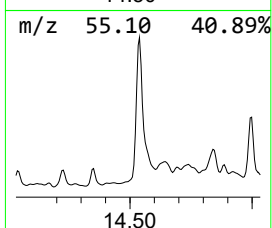
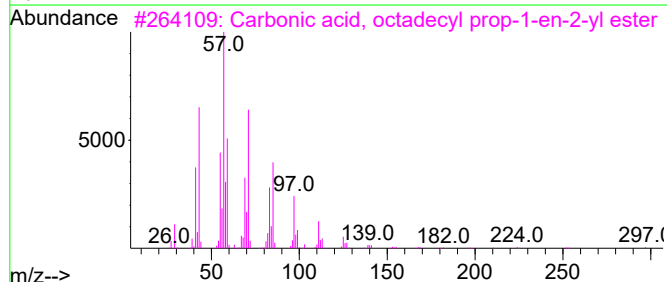
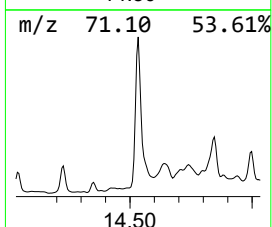
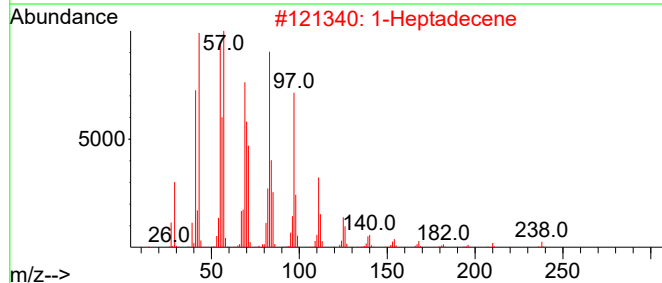
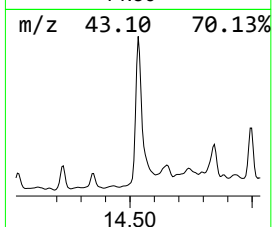
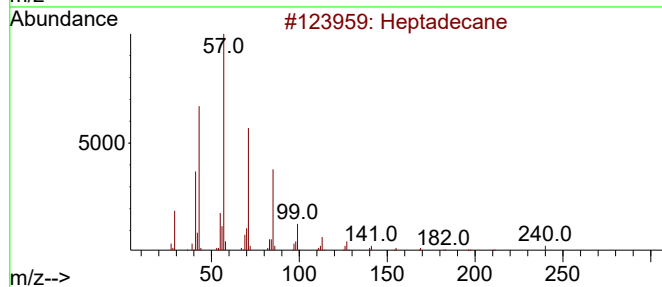
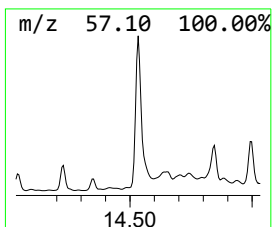
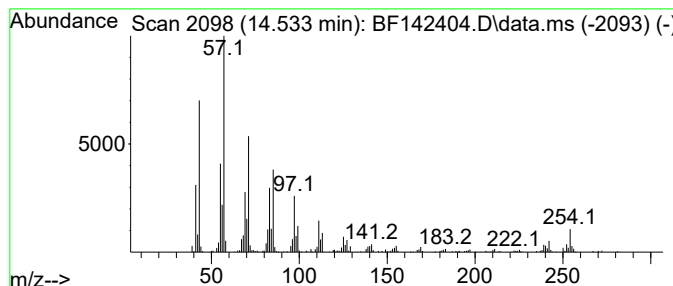
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.533	5.70 ng	371312	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	96
2			1-Heptadecene	238	C17H34	006765-39-5	94
3			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	90
5			Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142404.D
Acq On : 15 May 2025 21:05
Operator : RC/JU
Sample : Q2022-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

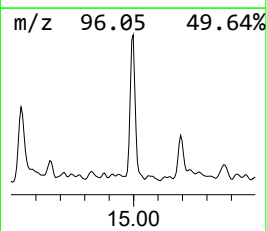
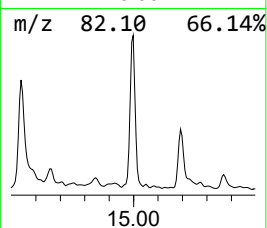
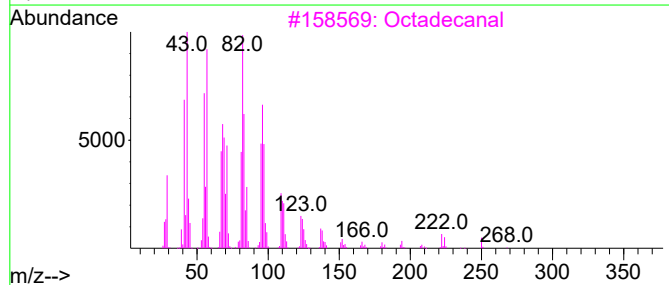
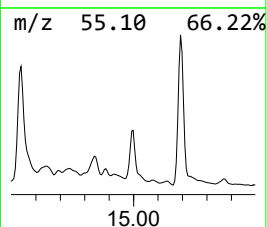
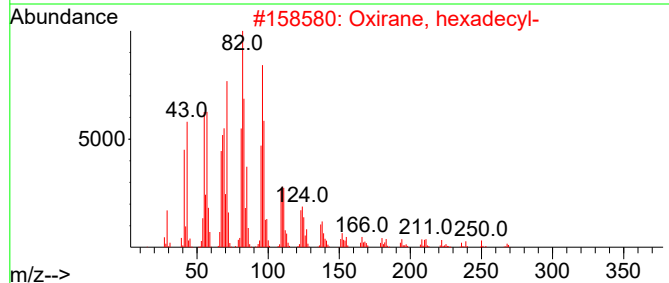
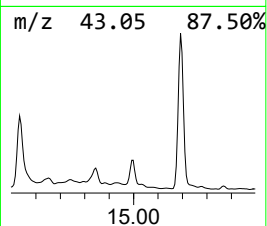
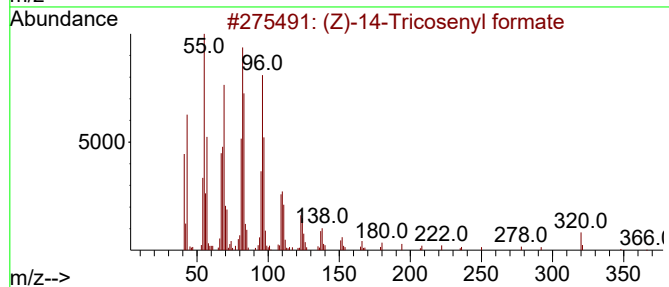
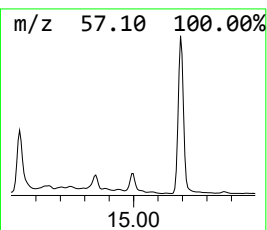
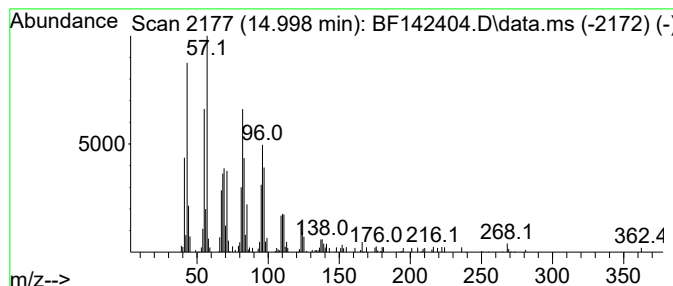
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (Z)-14-Tricosenyl formate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.998	4.64 ng	198675	Perylene-d12	15.551	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	90
3	Octadecanal	268	C18H36O	000638-66-4	90
4	1,19-Eicosadiene	278	C20H38	014811-95-1	86
5	Eicosanal-	296	C20H40O	002400-66-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142404.D
Acq On : 15 May 2025 21:05
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Sample : Q2022-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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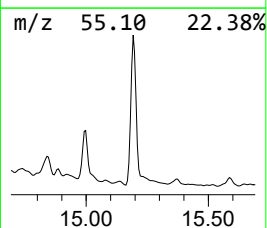
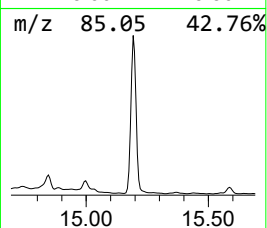
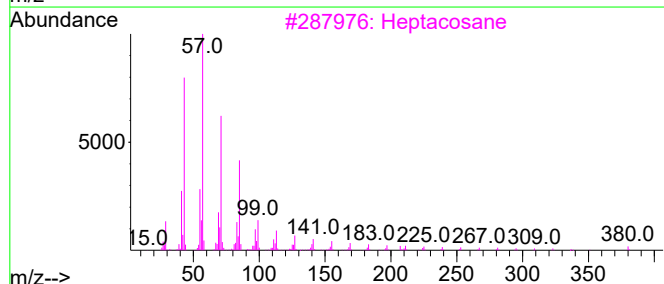
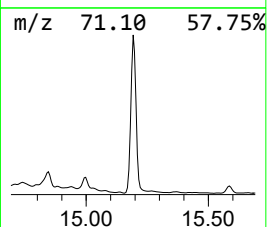
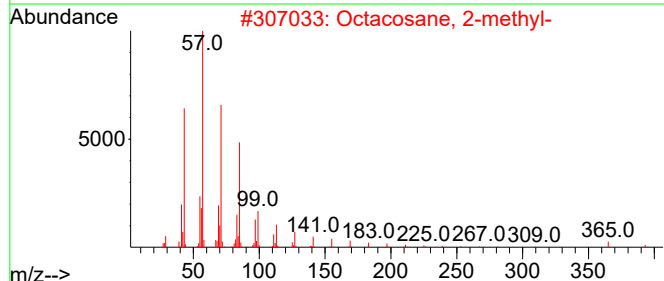
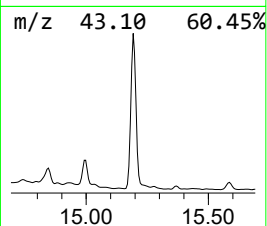
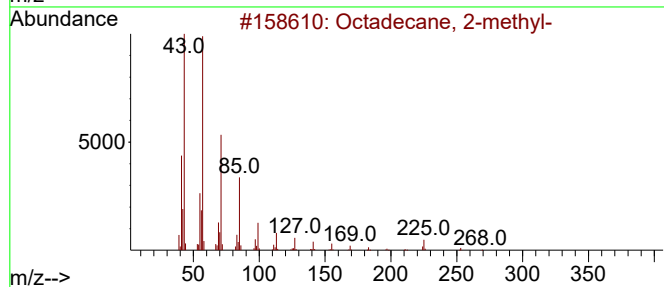
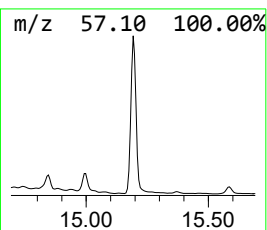
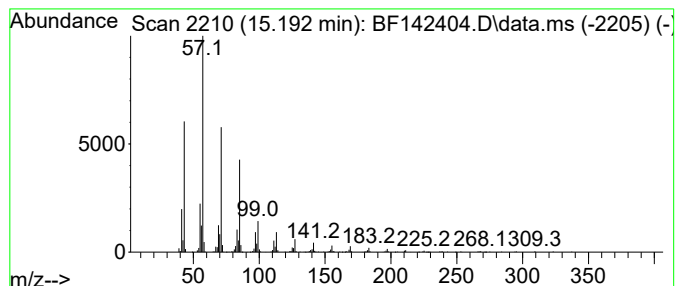
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.192	12.77 ng	546400	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93		
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91		
3	Heptacosane	380	C27H56	000593-49-7	91		
4	Heneicosane	296	C21H44	000629-94-7	91		
5	Octacosane	394	C28H58	000630-02-4	91		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142404.D
Acq On : 15 May 2025 21:05
Operator : RC/JU
Sample : Q2022-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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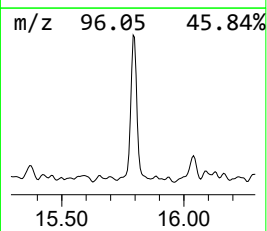
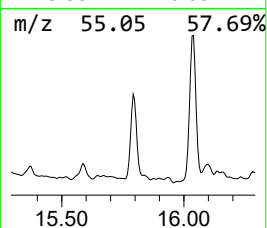
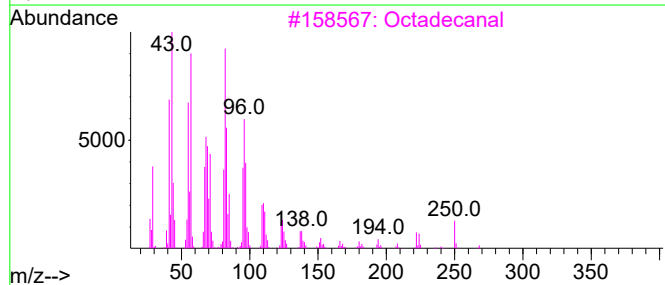
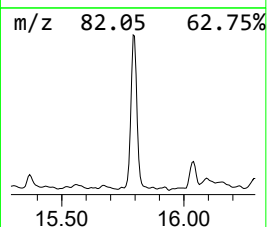
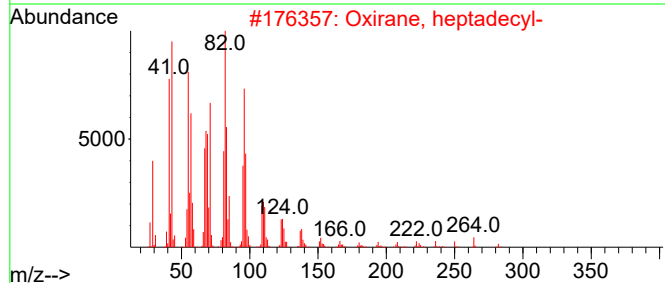
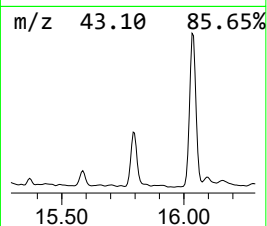
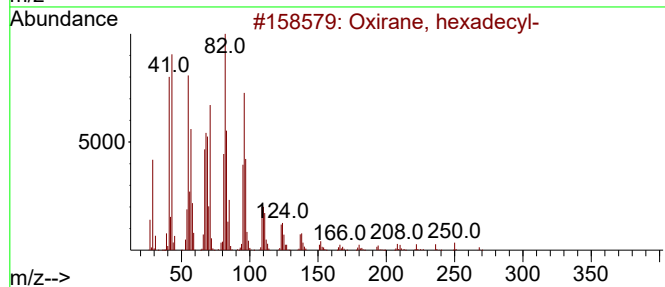
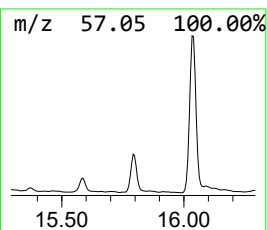
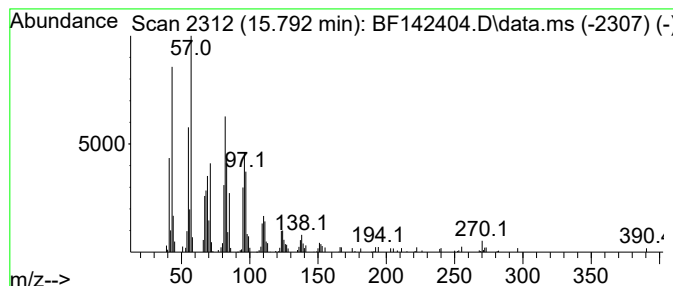
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.792	3.54 ng	151299	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	95
2			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	95
3			Octadecanal	268	C18H36O	000638-66-4	93
4			Tetracosanal	352	C24H48O	057866-08-7	87
5			Z-11,13-Dimethyl-11-tetradecen-1...	282	C18H34O2	1000131-36-6	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142404.D
Acq On : 15 May 2025 21:05
Operator : RC/JU
Sample : Q2022-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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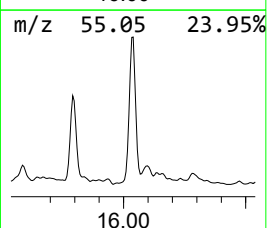
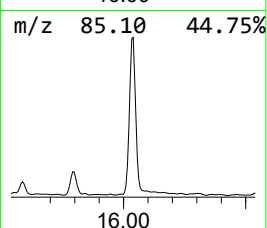
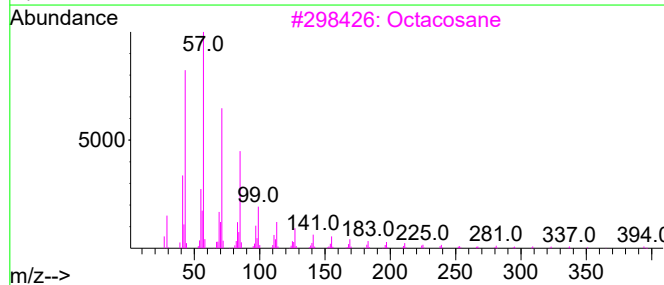
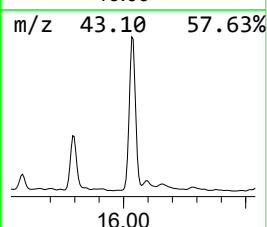
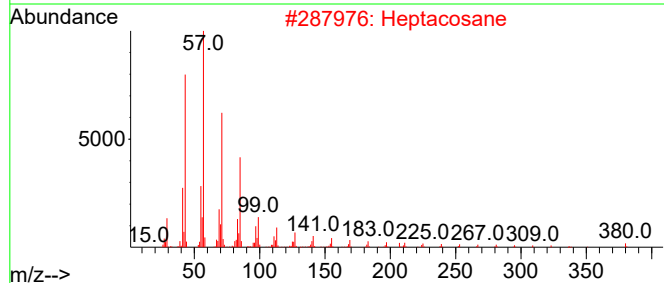
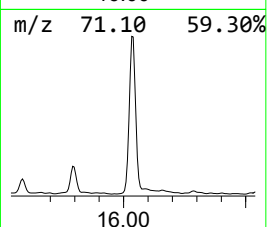
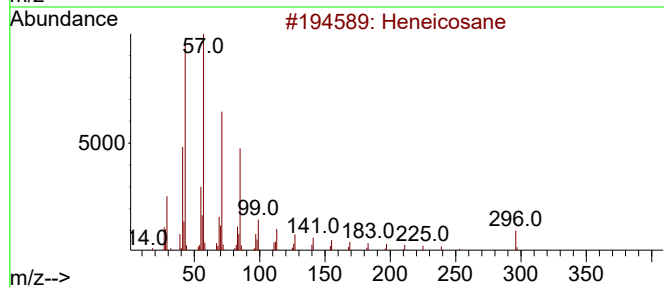
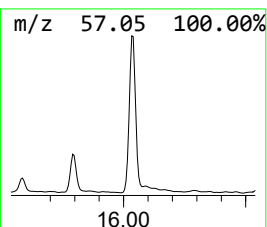
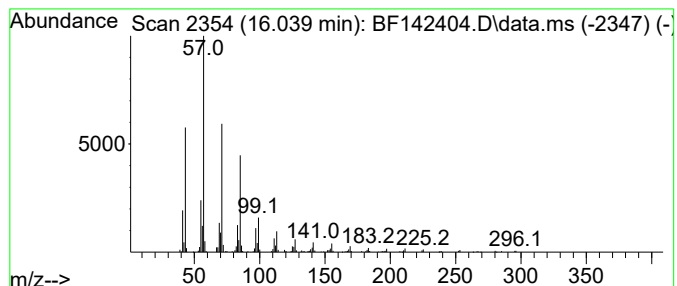
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.039	7.57 ng	323989	Perylene-d12	15.551

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heneicosane	296	C21H44	000629-94-7	95
2		Heptacosane	380	C27H56	000593-49-7	91
3		Octacosane	394	C28H58	000630-02-4	91
4		Tetratetracontane	619	C44H90	007098-22-8	91
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142404.D
Acq On : 15 May 2025 21:05
Operator : RC/JU
Sample : Q2022-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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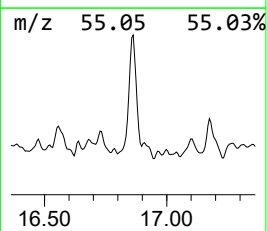
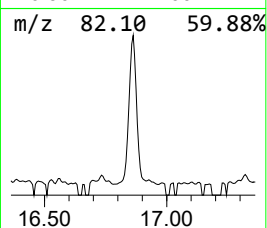
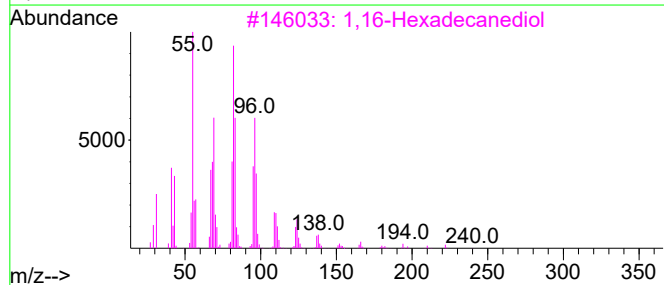
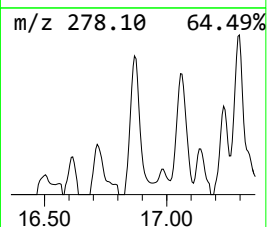
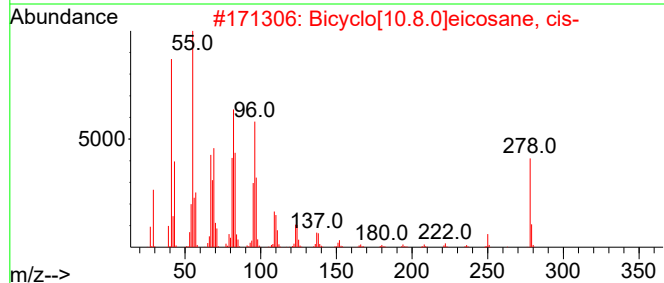
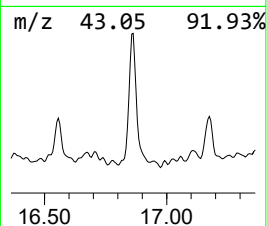
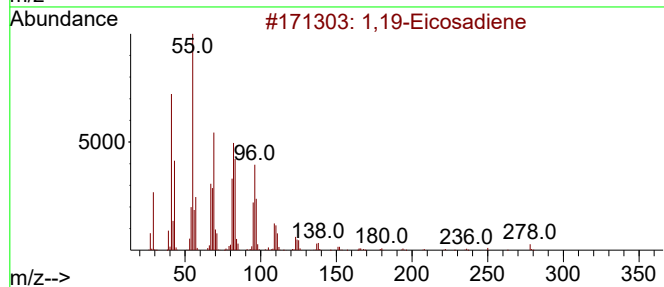
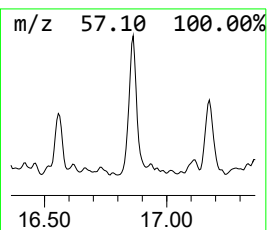
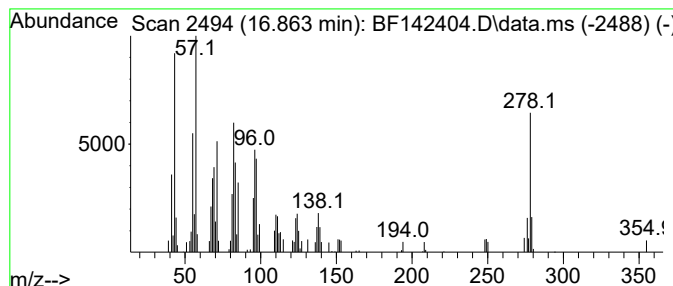
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 1,19-Eicosadiene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.863	2.06 ng	88041	Perylene-d12	15.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene			278	C20H38	014811-95-1	60
2	Bicyclo[10.8.0]eicosane, cis-			278	C20H38	1000155-82-2	58
3	1,16-Hexadecanediol			258	C16H34O2	007735-42-4	43
4	Cyclopentane, (4-octyldodecyl)-			350	C25H50	005638-09-5	43
5	Isobutyl octacosyl ether			467	C32H66O	1000406-33-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051525\
Data File : BF142404.D
Acq On : 15 May 2025 21:05
Operator : RC/JU
Sample : Q2022-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzophenone	10.651	8.5	ng	556707	3	9.934	1304180	20.0
n-Hexadecanoic ...	11.945	6.6	ng	461269	4	11.422	1392780	20.0
1-Dodecanol, 2-...	13.910	3.5	ng	231170	5	14.063	1302270	20.0
Heptadecane	14.533	5.7	ng	371312	5	14.063	1302270	20.0
(Z)-14-Tricosen...	14.998	4.6	ng	198675	6	15.551	855633	20.0
Octadecane, 2-m...	15.192	12.8	ng	546400	6	15.551	855633	20.0
Oxirane, hexade...	15.792	3.5	ng	151299	6	15.551	855633	20.0
Heneicosane	16.039	7.6	ng	323989	6	15.551	855633	20.0
1,19-Eicosadiene	16.863	2.1	ng	88041	6	15.551	855633	20.0